

Energy Dissipation and Fluctuation-Response in Driven Quantum Langevin Dynamics

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Abstract. – Energy dissipation in a nonequilibrium steady state is studied in driven quantum Langevin systems. We study energy dissipation flow to thermal environment, and obtain a general formula for the average rate of energy dissipation using an autocorrelation function for the system variable. This leads to a general expression of the equality that connects the violation of the fluctuation-response relation to the rate of energy dissipation, the classical version of which was first studied by Harada and Sasa. We also point out that the expression depends on coupling form between system and reservoir.

Introduction. – Recent developments in nonequilibrium statistical mechanics have clarified fundamental aspects of nonequilibrium fluctuations of work, power flux, heat absorbed etc [1–6]. The fluctuation theorem (FT) is one of the most remarkable discoveries in nonequilibrium statistical mechanics. This theorem quantifies the probability of negative entropy, which can be important for short measurement times in small systems, and provides a precise statement of the second law of thermodynamics. The relation between the transient version of FT and the Jarzynski equality has been demonstrated and clarified [5]. Both the FT and the Jarzynski relation [4] have been tested experimentally in systems, such as micromechanically manipulated biomolecules [7, 8], colloids in time-dependent laser traps [9, 10], and optically driven single two-level systems [11]. Studying robust properties valid in far-from-equilibrium regime is obviously important for understanding the general structures of nonequilibrium statistical mechanics.

Another important aspect of fluctuations is fluctuation-response. In the linear response regime, a fluctuation-dissipation relation (FDR) relates a response function with an auto correlation function for physical quantities at equilibrium [12–14]. However, the FDR is generically violated if the system is driven into a nonequilibrium state beyond this regime. Several recent studies considered extensions of FDR to far-from-equilibrium regime [15–17]. In Refs. [15, 16], the *violation function* was introduced to general-

ize the Einstein relation, and its validity was experimentally studied. Harada and Sasa considered the relationship between the degree of violation of FDR and the rate of energy dissipation in over-damped Langevin dynamics, and found *an equality valid in a far-from-equilibrium regime* [17]. The equality was first derived for the following

$$\gamma \dot{x}(t) = F(x(t), t) + \eta(t) + \varepsilon f(t), \quad (1)$$

where x are the coordinates, η is the white Gaussian noise satisfying $\langle \eta(t)\eta(u) \rangle = 2\gamma k_B T \delta(t-u)$, and $F(x(t), t)$ represents a force dependent on space and time. Let $C(t)$ be the autocorrelation function for the velocity fluctuation without perturbation, $\varepsilon = 0$

$$C(t) = \langle [\dot{x}(t) - v_s][\dot{x}(0) - v_s] \rangle, \quad (2)$$

where $\langle \dots \rangle$ denotes an ensemble average over thermal noise, and v_s is the average velocity of the particle. When the external perturbation is finite $\varepsilon \neq 0$, the response of the velocity obeys the linear response form [14]

$$\langle \delta \dot{x} \rangle = \varepsilon \int_{-\infty}^{\infty} dt' \chi(t, u) f(u). \quad (3)$$

Then the following equality was derived in Ref. [17]

$$I = \gamma \left\{ v_s^2 + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} [C(\omega) - 2k_B T \chi'(\omega)] \right\}, \quad (4)$$

where I is the rate of energy dissipation. $C(\omega)$ is the Fourier transformation of $C(t)$ and $\chi'(\omega)$ is the real part of the Fourier transformation of $\chi(t, u)$. In an equilibrium state with no dissipation flow $I = 0$, the FDR $C(\omega) = 2k_B T \chi(\omega)$ is satisfied. On the other hand, in a nonequilibrium state, the degree of violation of FDR is related to the rate of energy dissipation. This equality was generalized to correlated thermal noise by Deutsch and Narayan [18]. Recently an experimental test of Eq.(4) was performed in an optically driven colloidal system [19]. In general, it is difficult to conduct direct experimental measurements of energy dissipation flow. Eq.(4) suggests that the flow can be obtained with measurable functions in Langevin dynamics. Thus Eq.(4) is also of practical importance, providing a new protocol for measuring energy dissipation flow in driven Langevin dynamics.

In this paper, we consider a *driven quantum Langevin dynamics* and derive a wider class of relations that includes the quantum version of Eq.(4). Quantum Langevin dynamics has a wide variety of applications in areas such as electronic circuits, superconducting tunnel junctions, and electronic systems in semiconductors. [20]. Many different systems can be mapped onto a simple driven quantum Langevin equation. We derive a general relation, which reproduces the Callen-Welton FDR in an equilibrium state [21]. Our approach provides a unified method for investigating energy dissipation flow. This provides a new consideration of quantum energy dissipation with respect to Langevin dynamics, even if it includes nonlinear couplings between the system and the reservoirs.

Quantum Langevin Equation. – We consider a driven quantum Langevin system described as

$$\mathcal{H}(t) = \frac{p^2}{2m} + V(x, t) + \sum_{\ell} \left[\frac{p_{\ell}^2}{2m_{\ell}} + \frac{m_{\ell} \omega_{\ell}^2}{2} \left(x_{\ell} - \frac{\lambda_{\ell} x}{m_{\ell} \omega_{\ell}^2} \right)^2 \right]. \quad (5)$$

where $\{m, x, p\}$ refer to the system degrees of freedom, and $\{x_{\ell}, p_{\ell}, m_{\ell}, \omega_{\ell}\}$ refers to the reservoir. Those variables satisfy the commutation relations $[x, x_{\ell}] = [x_{\ell}, x_{\ell'}] = 0$, $[x, p] = i\hbar$, and $[x_{\ell}, p_{\ell'}] = i\hbar \delta_{\ell, \ell'}$. The potential term $V(x, t)$ drives the system into a nonequilibrium steady state. Detailed form is not provided here. The coupling constant between the system and bath oscillators $\{\lambda_{\ell}\}$ is switched on at time $t_{ini} = -\infty$. The initial density matrix is assumed to be of the product form $\rho_{ini} = \rho_S \otimes \rho_R$, where S and R refer to the system and the reservoir, respectively. These matrices are equilibrium distributions. The reservoir's density matrix is $\rho_R = e^{-\beta \mathcal{H}_R} / \text{Tr}[e^{-\beta \mathcal{H}_R}]$ for $\beta = 1/(k_B T)$. By eliminating the bath's degrees of freedom, we obtain a quantum Langevin equation easily [20], which is expressed as

$$m \frac{\partial^2 x}{\partial t^2} = -\frac{\partial V(x, t)}{\partial x} - \int_0^{\infty} du \gamma(u) \dot{x}(t-u) + \eta(t), \quad (6)$$

where η and $\gamma(t)$ represent a noise term and the memory kernels, respectively. These terms control dissipation effects from the bath. The properties of the noise and dissipation are completely determined by the initial condition of the bath. We define the spectral function

$$J(\omega) = \frac{\pi}{2} \sum_{\ell} \frac{\lambda_{\ell}^2}{m_{\ell} \omega_{\ell}} \delta(\omega - \omega_{\ell}). \quad (7)$$

Then, the dissipation kernels and noise correlations are given by

$$\begin{aligned} \gamma(t) &= \frac{2}{\pi} \int_0^{\infty} d\omega \frac{J(\omega)}{\omega} \cos \omega t, \\ \langle \eta(t) \eta(u) \rangle &= \frac{\hbar}{\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega(t-u)} \frac{\omega}{|\omega|} J(|\omega|) (1 + f(\omega)), \end{aligned}$$

where $f(\omega) = 1/(e^{\beta \hbar \omega} - 1)$. The Fourier transformation of the memory kernel is defined as $\gamma(\omega) = \int_0^{\infty} dt \gamma(t) e^{i\omega t}$. Then, the real part of the Fourier transformation $\gamma'(\omega)$ is expressed as

$$\gamma'(\omega) = J(|\omega|)/|\omega|. \quad (8)$$

Response Function. – In the Langevin dynamics, we consider the relationship between the response function and energy dissipation. The response function we consider is defined as the response of \dot{x} against a perturbation $-\varepsilon f(t)x$. The formal expression of response function $\chi(t, u)$ is calculated from the standard linear response derivation [14]. In the first order of ε , we obtain the deviation of density matrix from the unperturbed one as

$$\delta \rho(t) = \frac{-\varepsilon}{i\hbar} \int_{t_{ini}}^t du f(u) U(t, t_{ini}) [x(u), \rho(t_{ini})] U^{\dagger}(t, t_{ini}), \quad (9)$$

where $\rho(t)$ is the density matrix at time t , and $U(t, t_{ini})$ is the time-evolution operator defined as

$$U(t_f, t_i) = \exp_{\leftarrow} \left(-\frac{i}{\hbar} \int_{t_i}^{t_f} dt \mathcal{H}(t) \right). \quad (10)$$

The operator $x(u)$ is $U^{\dagger}(u, t_{ini}) x U(u, t_{ini})$. We take $t_{ini} \rightarrow -\infty$, and consider the deviation of the velocity \dot{x} which has the form (3). Then, we immediately obtain the response function, which is expressed using the retarded Green function $G_{xx}^r(t, u)$ as

$$\chi(t, u) = -G_{xx}^r(t, u) = \frac{i}{\hbar} \Theta(t-u) \langle [\dot{x}(t), x(u)] \rangle. \quad (11)$$

Here, $\langle \dots \rangle$ denotes an average over the initial state.

Energy Dissipation and the Callen-Welton FDR.

– We consider an energy dissipation flow from the system into the reservoir. By taking the derivative of the system's Hamiltonian with respect to time, we get the heat current operator

$$\mathcal{I} = -\sum_{\ell} \frac{\lambda_{\ell}}{m} p x_{\ell} + \sum_{\ell} \frac{\lambda_{\ell}^2}{2m_{\ell} \omega_{\ell}^2} \frac{1}{m} (x p + p x), \quad (12)$$

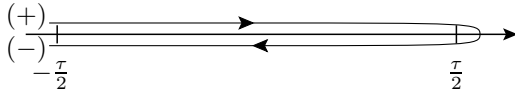


Fig. 1: Schwinger-Keldysh contour.

where positive current flows from the system into the reservoir. To arrive at the average current at the steady state, we employ the technique of Keldysh green function. We use conventional notations for the Green functions, which are defined for arbitrary operators, A and B , as

$$\begin{aligned} G_{AB}^k(t, t') &= -\frac{i}{\hbar} (\langle A(t)B(t') \rangle + \langle B(t')A(t) \rangle), \\ G_{AB}^{r,a}(t, t') &= -\frac{i}{\hbar} \Theta(\pm(t - t')) \langle [B(t), A(t')] \rangle, \end{aligned}$$

where $G_{AB}^k(t, t')$, $G_{AB}^r(t, t')$, and $G_{AB}^a(t, t')$ are the Keldysh, retarded, and advanced Green function, respectively. We set the initial time to be $t_{ini} = -\tau/2$. Using the green function, an average current is calculated as

$$I = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_{-\tau/2}^{\tau/2} dt \langle \mathcal{I}'(t) \rangle + I_0, \quad (13)$$

$$\langle \mathcal{I}'(t) \rangle = -\frac{i\hbar}{2} \sum_{\ell} \lambda_{\ell} \frac{\partial}{\partial t_1} G_{x, x_{\ell}}^k(t_1, t_2) \Big|_{t_1=t_2=t}, \quad (14)$$

where $I_0 = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_{-\tau/2}^{\tau/2} dt \frac{d}{dt} \langle x^2(t) \rangle \int_0^{\infty} d\omega \gamma'(\omega)/\pi$, which is the contribution from the second term in Eq.(12). We assume that the initial density matrix of the system is an equilibrium distribution for the Hamiltonian without the potential part $V(x, t)$, i.e., $p^2/2m + (x^2/2) \sum_{\ell} \lambda_{\ell}^2/(m_{\ell} \omega_{\ell}^2)$. This set up for initial state enables us to use the Wick theorem to compute the Green functions. Perturbation expansions for contour-ordered Green functions are performed along the Schwinger-Keldysh contour depicted in Figure 1. Using the Langreth rule for making the Keldysh Green function in Eq.(14) [22], we readily derive the average current

$$\begin{aligned} I &= I_0 + \lim_{\tau \rightarrow \infty} \frac{i\hbar}{2\tau} \int_{-\tau/2}^{\tau/2} \int_{-\tau/2}^{\tau/2} dt dt' \\ &\times \left\{ G_{xx}^r(t, t') \Sigma^k(t', t) + G_{xx}^k(t, t') \Sigma^a(t', t) \right\}. \end{aligned} \quad (15)$$

In Eq.(15), the function Σ^k and Σ^a are self-energy terms from the reservoirs, which calculated from the free green functions for reservoir's Hamiltonian. These are written as

$$\begin{aligned} \Sigma^k(t', t) &= \frac{-2i}{\pi} \int_0^{\infty} d\omega \gamma'(\omega) \frac{\omega}{\tanh(\frac{\beta\hbar\omega}{2})} \cos(\omega(t' - t)), \\ \Sigma^a(t', t) &= \frac{-2}{\pi} \Theta(t - t') \frac{\partial}{\partial t'} \int_0^{\infty} d\omega \gamma'(\omega) \cos(\omega(t' - t)). \end{aligned}$$

The formula (15) is valid for an arbitrary time-dependent

driving field. In order to simplify it further, we consider the following quantity for the Green function

$$G_{AB}^{\alpha}(\omega) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_{-\tau/2}^{\tau/2} \int_{-\tau/2}^{\tau/2} dt dt' G_{AB}^{\alpha}(t, t') e^{i\omega t} e^{-i\omega t'},$$

where α represents r, a , and k . When translational invariance in time is satisfied, this reduces to the usual expression of the Fourier transformation. Let $\chi'(\omega)$ denote $-\text{Re}[G_{xx}^r(\omega)]$. Then, a straightforward modification leads to

$$I = \frac{1}{\pi} \int_0^{\infty} d\omega \gamma'(\omega) \left[2\pi v_s^2 \delta(\omega) + C(\omega) - \frac{\chi'(\omega) \hbar \omega}{\tanh(\frac{\beta\hbar\omega}{2})} \right], \quad (16)$$

where we used the integral by parts to remove the term I_0 . Here, $C(\omega) = (i\hbar/2) G_{xx}^k(\omega) - 2\pi v_s^2 \delta(\omega)$, and v_s is the average velocity. In an equilibrium state where no net energy dissipation flow exists, the Callen-Welton FDR, $C(\omega) = \chi'(\omega) \hbar \omega / \tanh(\beta\hbar\omega/2)$ is satisfied [21]. In the limit $\hbar \rightarrow 0$ and by inserting $\gamma'(\omega) = \gamma$, the above equation reproduces Eq.(4).

Concluding Remarks. – Several general principles exist for nonequilibrium phenomena. In the linear response regime, the validity of the Onsager reciprocity and the Green-Kubo relations have been established. The fluctuation theorems and Jarzynski equality are being investigated in numerous models and experiments, and they seem to be the exact relations valid arbitrarily far from equilibrium. Eqs.(4) and (16) are also interesting, showing that the degree of FDR violation is related to energy dissipation in Langevin dynamics. This would be important, because Langevin dynamics is ubiquitous in realistic systems. Quantum Langevin dynamics is believed to have wide applicability in many realistic systems, including metallic tunnel junctions with capacitances and superconducting junctions [20, 23–25]. In those cases, the system and reservoir variables represent the variables in electrical circuits, and the external force is realized by an electric current. Circuit-realization of a driven harmonic trapped particle was proposed in Ref. [6]. The quantum case for this would be an interesting relevant system.

In the present study, Eq.(15) is the key equality for deriving the result (16). To derive Eq.(15), linear coupling between the system and thermal environment was critical. Although linear couplings should be the dominant contributions in most realistic systems, nonlinear couplings, where a nonlinear function of x couples with the bath variables, are also possible [26]. It is possible to generalize Eq.(15) to nonlinear coupling cases. In general, when we change the coupling form in the Hamiltonian (5) as $\lambda_{\ell} x_{\ell} x \rightarrow \lambda_{\ell} x_{\ell} f(x)$, a different expression of average current from Eq.(16) is obtained as

$$I = \frac{1}{\pi} \int_0^{\infty} d\omega \gamma'(\omega) \left[\frac{i\hbar}{2} G_{ff}^k(\omega) + \frac{\hbar \omega \text{Re}[G_{ff}^r(\omega)]}{\tanh(\frac{\beta\hbar\omega}{2})} \right]. \quad (17)$$

This means that the expression depends on types of coupling form. It would be important to figure out how Eqs. (4) and (16) are generalized, if we consider other types of reservoirs and dynamics. Energy dissipation of spin dynamics would be an important problem to be studied.

Another intriguing problem might be on higher order fluctuations of energy dissipation flow. Nonequilibrium fluctuations increases in time unlike equilibrium ones. To study characteristics of fluctuations, it is convenient to use the technique of counting statistics [27,28], which is equivalent to the protocol for obtaining *fluctuation theorem* in quantum systems [29–31] and work distribution [32]. It is possible to derive an explicit form of characteristic function, which generates not only average current but also any orders of cumulants of dissipation flow. It can reproduce the present result (16). Systematic derivatives of the characteristic function with respect to a counting field generates any orders of fluctuations. We hope that this study encourages further studies on energy dissipation at far-from-equilibrium conditions in quantum systems.

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